Supplemental Materials

Table S1. RMSDs of the backbone atoms in different segments of Bcl-xL in the simulations using different parameters with reference to the apo-Bcl-xL crystal structure (PDBID: 1MAZ).

Simulation System	α1 (4–18)	α2 (86–98)	α3 (104–111)	α4 (119–131)
1MAZ cMD	1.65 ± 0.38	1.24 ± 0.21	2.23 ± 0.86	1.84 ± 0.48
1MAZ low boost	1.94 ± 0.81	1.28 ± 0.25	3.89 ± 1.06	1.95 ± 0.65
1MAZ high boost	2.10 ± 0.37	1.45 ± 0.25	3.13 ± 0.87	2.72 ± 0.72
2BZW cMD	1.75 ± 0.34	0.82 ± 0.21	2.83 ± 1.00	2.39 ± 1.44
2BZW low boost	2.77 ± 1.19	1.43 ± 0.46	5.51 ± 2.44	2.57 ± 0.90
2BZW high boost	5.29 ± 2.44	1.56 ± 0.34	4.24 ± 0.95	3.62 ± 1.01
1MAZ cosolvent cMD	1.82 ± 0.44	1.40 ± 0.18	2.06 ± 0.67	1.73 ± 0.55
1MAZ cosolvent low boost	2.73 ± 0.87	0.95 ± 0.25	7.86 ± 2.13	8.61 ± 3.58
1MAZ cosolvent high boost	2.76 ± 1.42	1.83 ± 1.39	6.57 ± 1.88	4.96 ± 2.18
2BZW cosolvent cMD	1.08 ± 0.29	0.67 ± 0.14	3.60 ± 1.40	1.75 ± 0.67
2BZW cosolvent low boost	3.68 ± 1.75	1.98 ± 0.83	7.73 ± 1.77	5.39 ± 2.91
2BZW cosolvent high boost	2.46 ± 0.78	1.14 ± 0.40	8.38 ± 3.67	7.25 ± 3.43
Simulation System	α5 (137–156)	α6 (162–176)	α7 (188–192)	all (1–196)
1MAZ cMD	0.78 ± 0.11	1.64 ± 0.40	2.23 ± 0.54	1.99 ± 0.27
1MAZ low boost	0.78 ± 0.17	1.30 ± 0.44	1.84 ± 0.60	2.23 ± 0.30
1MAZ high boost	1.07 ± 0.19	1.85 ± 0.63	4.21 ± 1.44	3.33 ± 0.51
2BZW cMD	0.68 ± 0.12	1.10 ± 0.34	1.14 ± 0.58	1.97 ± 0.56
2BZW low boost	0.92 ± 0.19	1.34 ± 0.57	1.69 ± 0.92	2.68 ± 0.65
2BZW high boost	1.85 ± 0.57	3.73 ± 1.74	4.69 ± 1.59	4.71 ± 1.00
1MAZ cosolvent cMD	0.70 ± 0.16	1.79 ± 0.44	1.60 ± 0.56	2.05 ± 0.31
1MAZ cosolvent low boost	1.44 ± 0.28	3.87 ± 3.08	3.33 ± 1.69	5.61 ± 1.84
1MAZ cosolvent high boost	1.96 ± 1.06	3.42 ± 2.08	5.70 ± 3.66	5.10 ± 1.86
2BZW cosolvent cMD	0.68 ± 0.10	1.15 ± 0.39	1.61 ± 0.50	1.95 ± 0.46
2BZW cosolvent low boost	1.92 ± 0.85	3.78 ± 1.85	8.97 ± 5.09	5.64 ± 1.94
2BZW cosolvent high boost	1.26 ± 0.38	2.85 ± 1.04	5.17 ± 3.08	5.51 ± 1.73

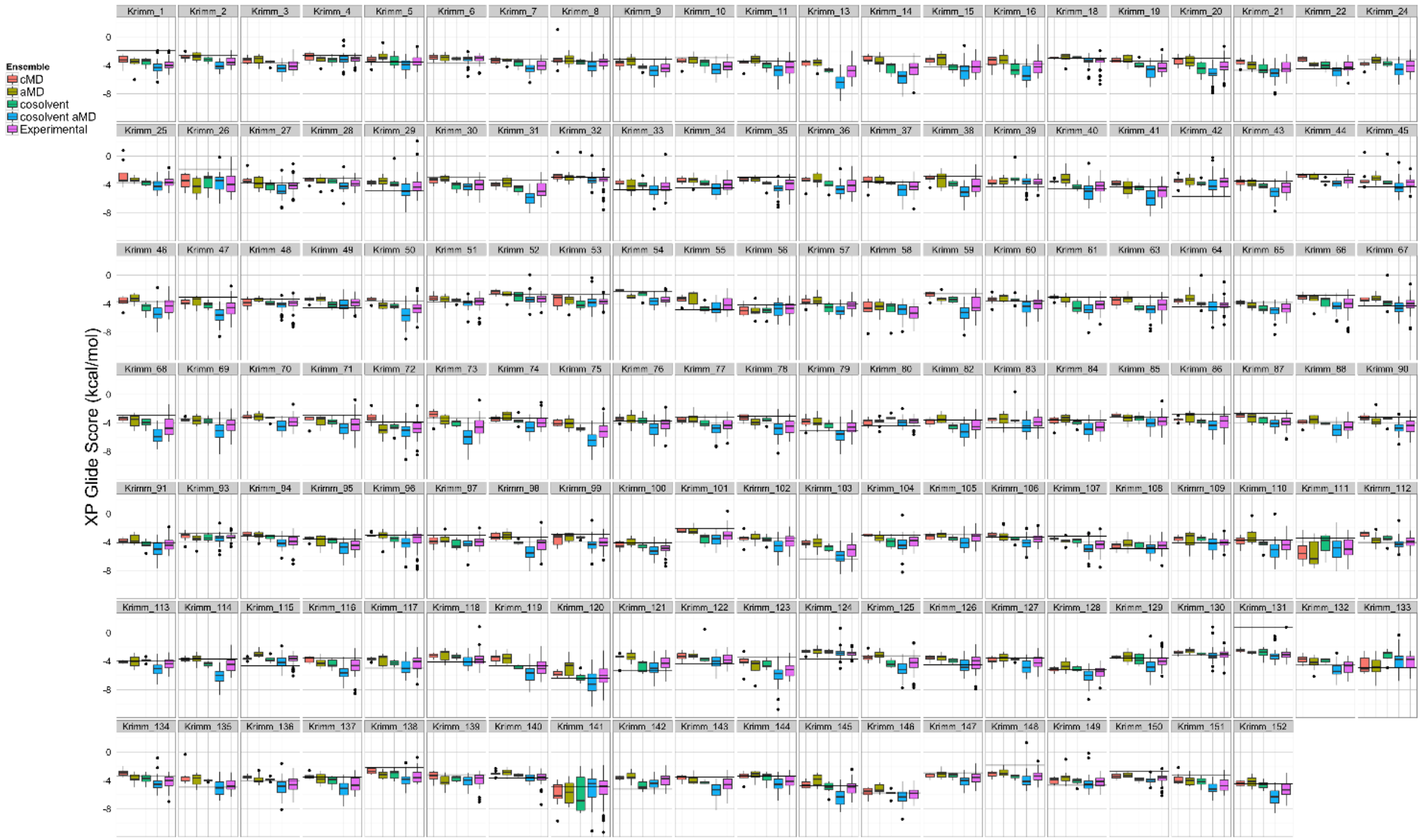

Figure S1. 145 decoys docked against the simulated and experimental structure ensembles.